Consortium for Advanced Modeling of Particle Accelerators (CAMPA)

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Vision:

- CAMPA, a national consortium and world leader for advanced modeling of particle accelerators, coordinates and integrates the development, maintenance, distribution and support of state-of-the-art accelerator computer codes. It advances accelerator science through advanced computation, in support of the Department of Energy's mission.

Mission:

- push the frontier of accelerator science through advanced simulation and modeling; push the computing frontier in accelerator science through algorithmic advances;
- provide the scientific community with a comprehensive and integrated toolset of state-of-the-art simulation codes for multi-scale, multi-physics accelerator modeling, in support of the mission of the Office of Science within the Department of Energy (DOE);
- develop and maintain the codes on DOE's supercomputing facilities; distribute and support codes for installation on smaller scale clusters, desktops or laptops;
- support users;
- use the codes as education tools to train students and young researchers on the science and the modeling of accelerators;
- promote collaboration and re-use of accelerator simulation codes and data through common interfaces, data standards, and integrated visualization and analysis capabilities;
- establish a framework aimed at its extension to a national consortium (short term).

Strategy:

- (long term) create a national consortium composed of a cohesive team of accelerator physicists, computational scientists and applied mathematicians from national labs and universities;
- (short term) create a core collaboration by assembling a cohesive team of accelerator physicists, computational scientists and applied mathematicians from LBNL, SLAC and FNAL;
- integrate the existing codes into a coherent toolset:
  - develop a unified easy-to-use set of graphical- and scripting-based front-ends and integrated scientific data analysis, visualization, and workflow software,
  - reduce duplication by promoting modularity, interoperability, re-use, and consolidation;
- support codes on existing computing hardware and on upcoming heterogeneous platforms encompassing emerging technologies such as GPU, MIC or others;
- support users through workshops, web-based resources (including documentation and help desk), as well as free and fee-for-service consultations in modeling of accelerator applications;
- use codes to understand and optimize existing accelerators, validate accelerator concepts,and designs, and to help develop, design, and engineer future accelerators with higher performance and lower cost;
- add new functionalities as dictated by application needs;
- teach at the US Particle Accelerator School and other relevant venues;
- take advantage of, and partner with, local and national resources (NERSC, SciDAC, ASCR funded programs, INCITE, etc.) as well as industry (through SBIR, STTR, etc.).

Scientific demand:

The vision, mission and strategy of CAMPA are consistent with the recommendations for the HEP accelerator simulation activities as given in the Report of the Particle Physics Project Prioritization Panel, May 2014 [1], the report from the Topical Panel Meeting on Computing and Simulations in High Energy Physics [2], and the summary of "Computing Frontier: Accelerator Science" from DOE's Community Summer Study Snowmass 2013 [3]. We detail in this section the relevance of CAMPA with regard to the related P5 recommendations:

- ***Recommendation 29: Strengthen the global cooperation among laboratories and universities to address computing and scientific software needs, and provide efficient training in next-generation hardware and data-science software relevant to particle physics. Investigate models for the development and maintenance of major software within and across research areas, including long-term data and software preservation.***
  For DOE-HEP accelerator activities that rely on complex computer modeling, CAMPA will provide an integrated set of accelerator simulation software that will speed up design and innovation in accelerator technologies. Unlike existing software developed by individuals inside projects, the CAMPA software suite will be developed and supported by a specialized and experienced team. This will consolidate scattered efforts to enable routine virtual prototyping of accelerator components on much larger scales than would be possible otherwise, leading to high payoffs that will maximize DOE-HEP return on investment.

- **p. 46:** ***"To address the science Drivers, increasingly higher demands are being placed on the performance in all three areas (accelerators, instrumentation and computing), at reduced cost. This necessitates the ongoing pursuit of innovation."***
  CAMPA's code development teams have an outstanding track record in innovative algorithms and use of high-performance computing. As a result, CAMPA's codes contain a remarkably large number of novel algorithms (including the "Lorentz boosted frame" approach) that were introduced by the developers and adopted elsewhere (see also Appendix C). The culture of innovation that permeates the CAMPA team will be a key asset for addressing the multiple challenges that will arise with the consolidation of code suites, the addition of new physics, and the porting of codes to emerging platforms.

- **p. 48:** ***"the use of high-performance computing, combined with new algorithms, is advancing full 3 -D simulations at realistic beam intensities of nearly all types of accelerators. This will enable "virtual prototyping" of accelerator components on a larger scale than is currently possible."***
  CAMPA's consolidation of modeling efforts and improved user support will enable routine virtual prototyping and modeling of virtual accelerators on a scale that is currently unavailable. Advances in accelerator computing advance both enablers: computing and accelerators. As advances in algorithms and codes will speed up advances in accelerator research, funding accelerator computing activities will have compounding effects.

Impact:

Thanks to sustained advances in hardware and software technologies, computer modeling is playing an increasingly important role in all areas of science and technology, and this trend is expected to continue for the foreseeable future. In application to the design of particle accelerators, this rise in importance is further fueled by the economic pressure for reducing uncertainties and costs in the development, construction, and commissioning of accelerators, thus pushing the field toward an increase use of "virtual prototyping", and ultimately towards code suites capable of modeling "virtual accelerators" to achieve machine optimization and design objectives at lower cost. In light of this, it is desirable to strengthen and coordinate programmatic activities of particle accelerator modeling within the HEP community [1-3]. This increased focus on computational activities is all the more timely as computer architectures are transitioning to new technologies that require the adaptation of existing - and emergence of new - algorithms and codes [4,5].

Through its new and unique mission in the DOE Office of Science, CAMPA will address several important issues that were raised in the reports [1-3], most notably the poor coordination of scattered modeling efforts and the lack of dissemination and effective usage of accelerator modeling tools. CAMPA will consolidate efforts from leading teams at three national laboratories (LBNL, SLAC, and Fermilab) who will merge and morph their existing modeling capabilities into a cohesive toolset. The collaboration will increase efficiency and free resources that will allow the development of more capabilities and user support. It will also enable users to simulate complex problems involving both electromagnetic and beam dynamics calculations together, which cannot be done with any existing package. By improving the cohesion of the existing development efforts and by ensuring that the codes are adequately disseminated and supported on DOE's supercomputing facilities, CAMPA will fulfill a central mission that will complete the DOE Office of Science portfolio in accelerator modeling activities (Fig. 1-a). The integration of accelerator physicists with applied mathematicians and computer scientists into a coherent team will enable the development of more capable codes with better algorithms that include more physics, thus accelerating the pace of advances in accelerator science (Fig. 1-b). The combined increase in codes, capabilities, dissemination, and support will significantly raise the impact – and thus the return on investment – of computer modeling on accelerator science and technology.

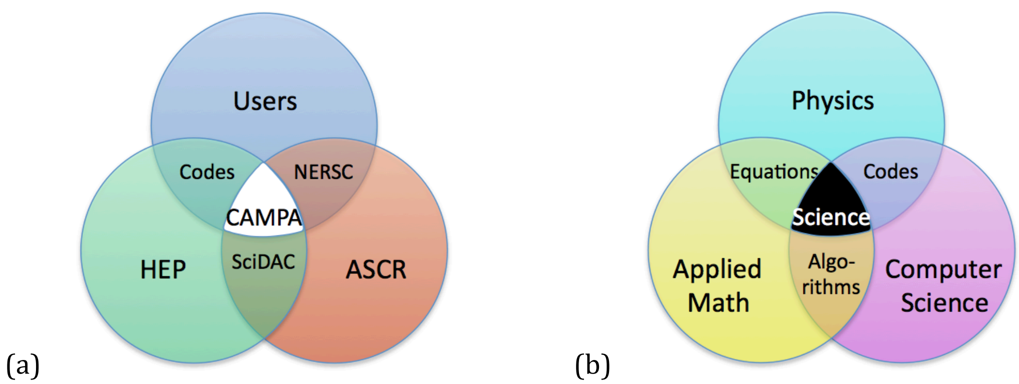

Fig. 1: (a) CAMPA will fulfill a central mission that will complete the DOE Office of Science portfolio in accelerator modeling activities. This new mission will significantly augment the impact – and thus the return on investment – of computer modeling on accelerator science and technology; (b) The integration of accelerator physicists with applied mathematicians and computer scientists into a coherent structure will enable the development of more capable codes with better algorithms that include more physics, thus accelerating the pace of advances in accelerator science.

The establishment of CAMPA will provide an outreach platform to introduce or enhance the use of high-performance computing (HPC) in electromagnetic and beam physics simulation to potential customers beyond the DOE accelerator complex. The tools that are developed for accelerator science are applicable to environment, industry, medicine, material science and other areas of national interests. The efforts of code integration, novel functionality development, and easy access for users endorsed by CAMPA will benefit many application areas, such as, plasma physics applications in fusion, astrophysics, spacecraft charging and propulsion, discharges, etc., as well as electromagnetic modeling for power sources, communication systems, antennas, radar, etc.

Uniqueness:

CAMPA's set of codes (see appendix A) constitutes a combination with a unique breadth for the modeling of beam dynamics and electromagnetics in particle accelerators. Combining HPC, advanced computational algorithms, and relevant physics, these codes provide a unique modeling and simulation capability to the accelerator community that is unmatched by existing efforts in the commercial and academic sectors. These codes have enabled the design of accelerators to high accuracy without the need for experimental tuning (thus saving costs) [6], contributed to discovery science in accelerators through advanced modeling (thus ensuring machine operation reliability) [7] and even to the discovery of new physics [8]. With application to linacs, rings, transfer lines, light sources, RF structures, injectors, particle traps, high-gradient structures (including dark currents), electron cloud effects, dielectric laser, and plasma-based accelerators, these codes have a wide user base with users distributed at over 50 institutions worldwide, including in the United States, Europe and Asia.

Most of CAMPA's codes were developed in part, and sometimes almost entirely, under the SciDAC program and have been instrumental to its success. In fact, CAMPA's codes had a leading or key role in all six of the key accomplishments that were listed in the final SciDAC-2 ComPASS report (see full report for more details):

1. boosted frame technique [9] (developed in WARP; reproduced in Osiris & Vorpal);
2. modeling of electron cloud effects for Project X and SPS (Synergia, WARP-POSINST);
3. end-to-end simulation of the ILC cryomodule (ACE3P);
4. laser plasma acceleration modeling (WARP & Vorpal – collaboration w/ Tech-X);
5. increased luminosity in Tevatron Run II program (BeamBeam3D);
6. modeling of Mu2e's debuncher (Synergia).

Integration of existing and emerging accelerator modeling tools, and their centralized support with users from the accelerator community at large, are defining missions of the new collaboration. Until now, the development of accelerator codes has been left to projects without mandate for coordination nor distribution or support. The new consortium will fill the current gap between the users, the codes, and the computing facilities. The SciDAC ComPASS collaboration effort develops and applies targeted codes on massively parallel supercomputers but does not provide user support nor code integration. The consortium will complement ComPASS' focus on high-performance computing by extending the support to lower-end computer platforms (such as clusters, desktops, or laptops) to broaden the access of users to using the codes. The partnership between accelerator physicists, computer scientists, and applied mathematicians endorsed by SciDAC will play an important role for the consortium as well, with additional emphasis on code integration. This will augment functionalities through developments based on code integration, such as accelerator optimization, that involve multiphysics arising from different components of the code suite.

CAMPA's codes constitute a very complementary set that contains the widest variety of models that is available in the community (see Appendix B). Such a complete set allows for covering the breadth of needs for accelerator modeling, as described in the previous section and in [1-3]. Furthermore, the developers of CAMPA's codes have demonstrated successes in addressing simulation and modeling challenges by pushing the computing frontier in accelerator science through algorithmic advances. As a result, the set of codes contains a remarkably large number of novel algorithms that were introduced by the developers and adopted elsewhere (see Appendix C). The culture of innovation that permeates the team will be a key asset for addressing the multiple challenges that will arise when integrating the code suite, adding new physics and porting the codes to emerging platforms.

References:

[1] Report of the Particle Physics Project Prioritization Panel, May 2014

[2] "Computing in High Energy Physics", Report from the Topical Panel Meeting on Computing and Simulations in High Energy Physics, 2014

[3] "Computing Frontier: Accelerator Science", P. Spentzouris *et al.*, DOE's Community Summer Study Snowmass 2013; http://arxiv.org/abs/1310.2203;

[4] J. Shalf, J. Bashor, D. Patterson, K. Asanovic, K. Yelick, K. Keutzer and T. Mattson, "The Manycore Revolution: will HPC Lead or Follow?," SciDAC Review (2009); http://www.scidacreview.org/0904/html/multicore.html

[5] J. Cohen, C. Cantwell, N. C. Hong, D. Moxey, M. Illingworth, A. Turner, J. Darlington and S. Sherwin, "Simplifying the Development, Use and Sustainability of HPC Software," (2013); http://arxiv.org/pdf/1309.1101.pdf

[6] J. Siegrist, Report from DOE/HEP, High Energy Physics Advisory Panel, Washington, D,C,, March 12-13, 2012, http://science.energy.gov/~/media/hep/hepap/pdf/march-2012/Siegrist_FY13_HEPAP_Briefing_JS_v2a_March_12.pdf, slide 27.

[7] M. Strayer, SciDAC Update, SciDAC 2010 Conference, July 11-15, Chattanooga, Tennessee, http://computing.ornl.gov/workshops/scidac2010/presentations/m_strayer.pdf, slide 15.

[8] "Ping-Pong modes: a new form of multipactor," R.A. Kishek, *Phys. Rev. Lett.* 108, 035003 (2012).

[9] http://science.energy.gov/hep/highlights/2013/hep-2013-04-a;
http://science.energy.gov/news/in-focus/2011/04-21-11-s;
http://focus.aps.org/story/v19/st10

Appendix A: Initial set of CAMPA Codes

Electromagnetics

Advanced Computational Electromagnetics 3P (ACE3P) suite (SLAC): 3-D frequency and time domain parallel finite-element electromagnetic (EM) and Particle-In-Cell (PIC) codes as well as multi-physics codes including integrated electromagnetic, thermal and mechanical effects for the modeling of accelerator cavities and structures. ACE3P includes:

- Omega3P (complex eigenvalue solver for finding the normal modes in an RF cavity),
- S3P (s-parameter solver to calculate the transmission in open structures),
- Track3P (particle tracking code with surface physics to study multipacting and dark current),
- T3P (time-domain solver for transient response to driven fields & beam excitations of wakefields),
- Pic3P (PIC code to simulate self-consistent electrodynamics of charged particle beams)
- TEM3P (Multi-physics module to perform integrated EM, thermal & mechanical analysis.)

Beam dynamics emphasizing linacs, beam-beam/medium interactions, advanced accelerators

Berkeley Lab Accelerator Simulation Toolkit (BLAST) suite (LBNL): 2-D and 3-D finite-difference and spectral electrostatic/electromagnetic Particle-In-Cell codes for the modeling of beam dynamics in particle accelerators, including beam-beam effects, electron clouds, collisions, emission from surfaces and laser-plasma acceleration. The BLAST suite includes:

- BeamBeam3D (3-D parallel electrostatic PIC for the modeling of strong-strong or strong-weak beam-beam interactions in high energy colliders),
- IMPACT suite (3-D parallel electrostatic PIC framework for modeling high intensity, high brightness beams in accelerators [Combination of MaryLie includes both high order optics based on Lie algebraic maps along with parallel 3D space-charge effects]),
- POSINST (2-D electrostatic PIC code for electron cloud buildup studies with detailed secondary electron yield module)
- WARP (2-D and 3-D parallel electrostatic and electromagnetic PIC general framework for modeling of particle beam generation, transport in accelerator lattice, neutralization in plasma, laser-plasma acceleration, etc. [combination with Posinst enables fully self-consistent electron cloud effects studies]).

Beam dynamics emphasizing circular accelerators and long-term tracking

Synergia (Fermilab): hybrid Python/C++ package for single or multiple bunch accelerator simulations utilizing PIC methods. Synergia includes fully nonlinear and symplectic independent-particle physics, as well as symplectic linear maps, arbitrary-order polynomial maps and non-linear map analysis, as well as collective effects, including space charge and wake fields, in various approximations ranging from the very simple to computationally-intense, 3-dimensional field calculations. Synergia's scriptable interface allows for arbitrary logical and ramping operations during the course of a simulation.

Appendix B: List of models

Fields:

- electrostatic and magnetostatic
  - multigrid
  - spectral
  - internal conductors
- electromagnetic
  - finite-difference (arbitrary order; nodal and staggered)
  - finite-element
  - non-standard-finite-difference
  - spectral
  - Perfectly Matched Layer absorbing boundary
  - internal conductors
  - finite conductivity, permittivity and permeability
- adaptive mesh refinement

Particles:

- pushers
  - leapfrog ‘Boris’
  - Runge-Kutta
  - Lorentz invariant
  - hybrid drift-Lorentz
  - implicit Newmark-beta
  - transfer map
- emission & collisions
  - space charge limited, thermionic, field, hybrid or arbitrary
  - secondary electron emission, ion-impact electron and gas emission
  - ionization, capture, charge exchange

Solvers:

- time domain (t-based)
  - lab frame
  - moving window
  - boosted frame
- slice (s-based)
- frequency domain (for RF cavities)
- iterative (for injector design)
- build-up (for study of electron cloud build-up)
- quasi-static

Accelerator lattices:

- High-order mapping
- solenoids, dipoles, quadrupoles, sextupoles, arbitrary fields, etc
- MAD file readers

Appendix C: algorithms invented, improved or pioneered in CAMPA's codes.

Algorithm/method	Reference	Originated	Adopted by
Parallel finite-element frequency domain eigensolver	*Zhan, Stanford Ph.D. thesis 1998*	ACE3P	
Stochastic Leap-Frog for Brownian motion	*Qiang & Habib, PRE 2000*	IMPACT	
Spectral-finite difference multigrid solver	*Qiang & Ryne, CPC 2001*	IMPACT	
Improved Perfectly Matched Layers	*Vay, JCP 2000/JCP 2002*	Warp	Osiris
AMR-PIC electrostatic	*Vay et al., LPB2002*	Warp	
Filter algorithm for large-scale eigenvalue problems	*Sun, Stanford Ph.D. thesis 2003*	ACE3P	
Visualization of large, complex line-based datasets	*Schussman, UC Davis Ph.D. thesis 2003*	ACE3P	
Secondary emission of electrons algorithm	*Furman & Pivi, PRST-AB 2003*	Posinst	TxPhysics, Warp, spacecraft charging codes
AMR-PIC electromagnetic	*Vay et al., CPC 2004*	Emi2D	Warp
3D Poisson solver with large aspect ratio	*Qiang & Gluckstern, CPC 2004*	IMPACT	
Shift-Green function method	*Qiang et al, CPC 2004*	BeamBeam3D	
Integrated Green function	*Ryne & Qiang*	ML/IMPACT BeamBeam3D,IMPACT	ASTRA, OPAL
Hybrid Lorentz particle pusher	*Cohen et al., NIMA 2007*	Warp	
Lorentz boosted frame	*Vay, PRL 2007*	Warp	INF&RNO, JPIC, Osiris, Vorpal
Explicit Lorentz invariant particle pusher	*Vay, PoP 2008*	Warp	Tristan, THISMPI, Photon-Plasma, PIConGPU
Parallel time domain and PIC in finite element	*Candel et al., ICAP 2009*	ACE3P	

Shape determination of accelerator cavities	*Akcelik et al., JCP 2009*	ACE3P	
Adaptive error estimators for electromagnetic field solvers	*Chen, Stanford Ph.D. thesis 2009*	ACE3P	
High-order FFT method for convolution integral w/ smooth kernel	*Qiang, CPC 2010*	N/A	
Mixed Particle-Field decomposition method	*Qiang & Li, CPC 2010*	BeamBeam3D	IMPACT, Synergia
Moving window technique in unstructured grid	*Lee et al., JCP 2010*	ACE3P	
PIC with tunable electromagnetic solver	*Vay et al., JCP 2011*	Warp	Vorpal, Osiris
Efficient digital filter for PIC	*Vay et al., JCP 2011*	Warp	Vorpal, Osiris
Domain decomposition for EM spectral solver	*Vay et al., JCP 2013*	Warp	

Appendix D: Summary of Snowmass report "Computing Frontier: Accelerator Science"

The Snowmass report [3] detailed the areas of applications of accelerator and beam physics modeling for the energy and intensity frontiers, ranging from conventional linacs and rings to advanced concepts such as plasma based accelerators, dielectric structures and muon colliders. It emphasized that modeling is an essential component of accelerator activities and that its importance is on the rise. It pointed out that there is a clear need for increasing the programmatic support of code development, as well as its coordination, targeting a reduction of duplication of code functionalities through increase in modularity and interoperability of components. Moreover, the proliferation of small "single physics" or "few physics" codes, often developed by a single accelerator physicist, is limiting progresses. Efforts to integrate more physics into codes are needed.

The future needs that are listed in the report call for larger codes with more physics and better algorithms that can run bigger problems on future cutting-edge supercomputers. Significant algorithm development is required to develop the codes that will exploit the upcoming supercomputer architecture based on heterogeneous hardware using GPU, MIC technologies or others to come. There is also a need for specialized algorithmic development that can enhance codes modeling functionalities to address current and future applications. These call for the establishment of an integrated team of computational physicists, computer scientists and applied mathematicians that is capable of carrying out the development of algorithms and codes to enable multi-physics modeling of challenging problems for accelerator and beam physics on emerging computer platforms.

Finally, it is noted that the current practice is less than optimal in that with few exceptions the users of High Performance Computing (HPC) accelerator codes are the developers, and that the scientific productivity would thus be enhanced by making the accelerator codes more widely usable. The adoption of the codes by the community would be greatly facilitated by supporting the development of community libraries and tools, including standardized user interfaces (scripting- or graphical-based), geometry and data descriptions, I/O, analysis and visualization tools. The development of generic workflow tools that perform in an HPC environment as well as local workstations and clusters is very important for the users. Similarly the development of parameter optimization libraries is in great demand. Furthermore, the use of scripting languages like Python for the development of standardized user interfaces can ease code integrations by minimizing disruption to current codes and practices while enabling both interoperability and expansion capabilities.